

# NIST Materials Resource Registry

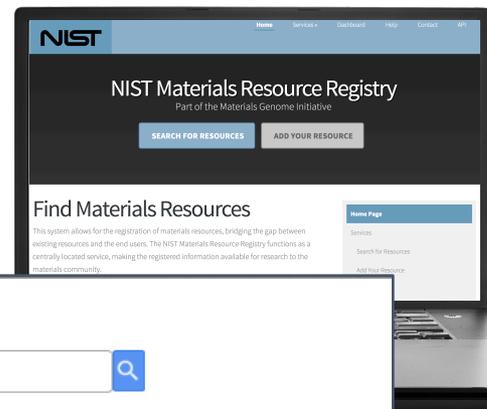
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NIST



# Materials Resource Registry

*As you heard in January...*

The NMRR is about making data discoverable



### Search for Resources

DFT \*

4 results

- All Resources
- Organizations
- Data Collections
- Datasets
- Services
- Informational Sites
- Software

Custom View

[Change Custom View](#)

Resource Type:

- All Resources
- Organization
- Data Collection
- Repository
- Project Archive
- Database
- Dataset
- Service
- Informational Site
- Software

MPIInterfaces <span>Resource Details</span> <span>Go To</span>	
title	MPIInterfaces
description	MPIInterfaces is a python package that enables high throughput Density Functional Theory (DFT) analysis of arbitrary material interfaces (ligand capped nanoparticles, surfaces in the presence of solvents and heterostructure interfaces) using VASP, VASPsol, LAMMPS, materialsproject database as well as their open source tools and a little bit of ASE.
subject	Python, Density Functional Theory (DFT), materials interfaces, surfaces, VASP, VASPsol, LAMMPS, MaterialsProject, ASE
referenceURL	<a href="http://henniggroup.github.io/MPIInterfaces/">http://henniggroup.github.io/MPIInterfaces/</a>
AFLOW <span>Resource Details</span> <span>Go To</span>	
title	AFLOW
description	Aflow is a globally available database of 647,815 material compounds

# Materials Resource Registry

*As you heard in January...*

The NMRR is a web application

- Collects descriptions of data resources
- Descriptions are searchable
- Ingesting descriptions:
  - Manually via web form
  - Programmatically via a REST interface
  - Harvest from data repositories or other registries
- Can operate in a federated environment of registry instances
- Can be adapted to any metadata schema (not specific to Materials Science)
- Supports a variety of Resource types:
  - Repositories,
  - Data collections (e.g. within repositories),
  - Databases, Services, Portals, Web sites,
  - Organizations



## Search for Resources

DFT

4 results



All Resources



Organizations



Data Collections



Datasets



Services



Informational

Custom View

Change Custom View

- Resource Type:
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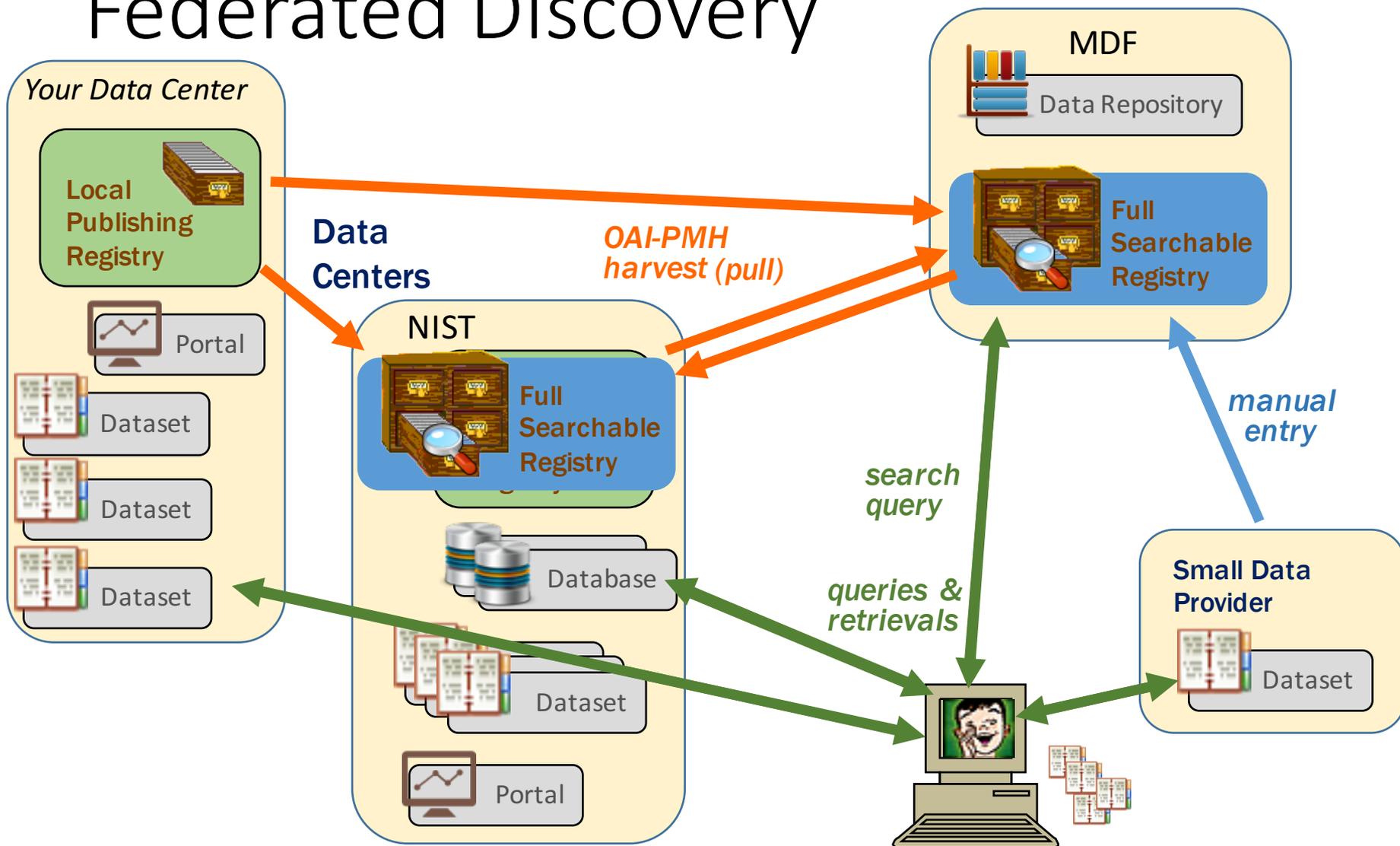
### MPInterfaces

title	MPInterfaces
description	MPInterfaces is a python package that enables high throughput Functional Theory (DFT) analysis of arbitrary material capped nanoparticles, surfaces in the presence of solvent structure interfaces) using VASP, VASPsol, LAMMPS, materials database as well as their open source tools and a little
subject	Python, Density Functional Theory (DFT), materials informatics, VASPsol, LAMMPS, MaterialsProject, ASE
referenceURL	<a href="http://henniggroup.github.io/MPInterfaces/">http://henniggroup.github.io/MPInterfaces/</a>



NIST Materials Genome Initiative

# Federated Discovery



# What should we register?

- Participate at various levels, depending on your available (people-time) resources
- Things to register
  - Your project/portal/web site (easy minimum)
  - Major data collections from your project
    - Describe the research aims and topics they address
  - Databases (and how one accesses them)
  - Repositories
    - might contain many smaller collections, each addressing a different research concern
    - Use one of the automated mechanisms to share descriptions
  - Software products
  - Services
- the question of granularity
  - Things not to register
    - Individual files
    - Records from a database
  - Can the data be described well by a unique abstract?



# How can we register things?

- One or a few ( $\lesssim 10$ ) resources?
  - Visit the registry at the Materials Data Facility (in progress)
  - Create an account and use web forms to describe your assets
- Many resources
  - Consider running your own registry
  - NMRR app can be run at your own site
  - REST API can be used to upload descriptions
  - Can connect it to your own information infrastructure



# How we describe our resources

- A materials-supporting schema is in development
  - Identity information – how we refer to it?
  - Provenance/Curation – who is responsible?
  - Description/Content metadata – what is it about?
  - Access information – how do we get at it?
  - Applicability metadata – how is it relevant to different communities?

Materials science, chemistry, physics, etc.



# How we describe our resources

Materials Resource Registry Curation System

141.142.209.111:8181/curate/enter-data?id=568ff6d78c2894d85c67639

MSMSE-IPR-2014.docx Thermodyna...up - Home Interatomic...ject - Home

## Resource

Local ID  
UKK8LPL6G0TAK9DEWC6W

Status  
Active

## Identity

Software Name MPInterfaces

Short Name MPInterfaces

Version +

Identifier +

Logo +

## Curation

Publisher  
Hennig group, University of Florida

PID:

Creator + -  
Arunima Singh

Materials Resource Registry Curation System

141.142.209.111:8181/curate/enter-data?id=568ff6d78c2894d85c67639

MSMSE-IPR-2014.docx Thermodyna...up - Home Interatomic...ject - Home

## Materials Science

Material Types

<input type="checkbox"/> polymer	<input checked="" type="checkbox"/> metal	<input checked="" type="checkbox"/> nanomaterials
<input type="checkbox"/> organic	<input checked="" type="checkbox"/> oxide	<input checked="" type="checkbox"/> inorganic
<input type="checkbox"/> composite	<input checked="" type="checkbox"/> semiconductor	<input checked="" type="checkbox"/> non-specific
<input checked="" type="checkbox"/> ceramic	<input type="checkbox"/> biomaterial	<input type="checkbox"/> superconductor

Morphology/Structures

<input checked="" type="checkbox"/> 2D	<input type="checkbox"/> amorphous	<input checked="" type="checkbox"/> non-specific
<input type="checkbox"/> fiber	<input type="checkbox"/> fluid	<input checked="" type="checkbox"/> crystalline
<input checked="" type="checkbox"/> interfacial	<input checked="" type="checkbox"/> bulk	<input type="checkbox"/> quasi-periodic
<input checked="" type="checkbox"/> interphase	<input type="checkbox"/> 1D	<input checked="" type="checkbox"/> film
<input checked="" type="checkbox"/> composite	<input type="checkbox"/> line defect	
<input type="checkbox"/> nanotube	<input type="checkbox"/> point defect	

Material Property Classes

<input checked="" type="checkbox"/> thermodynamic	<input type="checkbox"/> optical	<input type="checkbox"/> transport
<input checked="" type="checkbox"/> mechanical	<input checked="" type="checkbox"/> simulated	<input checked="" type="checkbox"/> structural
<input checked="" type="checkbox"/> defect	<input checked="" type="checkbox"/> non-specific	

Experimental Data Acquisition Methods

<input type="checkbox"/> electron microscopy	<input type="checkbox"/> impact testing	<input type="checkbox"/> scattering-diffraction
<input type="checkbox"/> indentation	<input type="checkbox"/> other	<input type="checkbox"/> load frame testing
<input type="checkbox"/> calorimetry	<input type="checkbox"/> spectroscopy	<input type="checkbox"/> optical microscopy
<input type="checkbox"/> atom probe microscopy	<input type="checkbox"/> dilatometry	<input type="checkbox"/> non-specific

Computational Data Acquisition Methods

<input type="checkbox"/> computational thermodynamics	<input type="checkbox"/> boundary tracking/level set	<input type="checkbox"/> non-specific
<input checked="" type="checkbox"/> numerical simulations	<input checked="" type="checkbox"/> density functional theory calculation	<input type="checkbox"/> crystal plasticity calculation
<input checked="" type="checkbox"/> molecular dynamics simulation	<input type="checkbox"/> multiscale simulations	<input type="checkbox"/> dislocation dynamics
<input type="checkbox"/> phase field calculation	<input type="checkbox"/> finite element analysis	
<input type="checkbox"/> statistical mechanics	<input type="checkbox"/> monte-carlo simulation	

Sample Processing Methods

# How we describe our resources

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  - Applicability metadata – how is it relevant to different communities?
    - Materials science, chemistry, physics, etc.
- Interested in participating in the schema development?
  - NIST and partners are collaborating on this via RDA Working Group
  - NIST will orchestrate migration of resource descriptions as schema evolves

